

Phase Command-Line Database Management and Searching

Database management tasks can be run in the foreground or submitted as a single-CPU job to any host that has access to the database directory. Site creation and database search jobs can be run on multiple processors. When you create the database, make sure that it is on a file system that is accessible to all hosts that need access to the database. For details on the commands and options, see [Chapter 13](#) of the *Phase User Manual*.

To create a new database:

```
$SCHRODINGER/utilities/phasedb_manage -new -db dbname {-mae maeFile|-sd sdFile} [-fd fdFile]
    -confs multiConfs [-ignoreTitles] [-unique propName] [-blimit maxMol] [job-options]
```

To add molecules to an existing database:

```
$SCHRODINGER/utilities/phasedb_manage -add -db dbname {-mae maeFile|-sd sdFile} -confs multiConfs
    [-ignoreTitles] [-unique propName] [-blimit maxMol] [job-options]
```

To restart a failed database creation or molecule addition:

```
$SCHRODINGER/utilities/phasedb_manage -db dbname {-mae maeFile|-sd sdFile} [-fd fdFile] -RESTART
```

To delete molecules from a database:

```
$SCHRODINGER/utilities/phasedb_manage -delete -db dbname -records recordFile [job-options]
```

To generate conformers and pharmacophore sites:

```
$SCHRODINGER/utilities/phasedb_confsites -db dbname [-sub dbSubset] -JOB jobname [-RESTART]
    [-BLOCK m] [job-options] [-confs {auto|all}] [-max maxConfs] [-ewin deltaE]
    [-sample {rapid|thorough}] [-amide {orig|vary|trans}]
```

To restart a conformer and site generation job:

```
$SCHRODINGER/utilities/phasedb_confsites -db dbname -JOB jobname [job-options] -RESTART
```

To create a subset from the structures in a hit file:

```
$SCHRODINGER/utilities/phasedb_subset -db database -hits hitfile -out subset
```

To create a subset from a logical operation on two existing subsets:

```
$SCHRODINGER/utilities/phasedb_subset -db database -in1 subset1 -logic {AND|OR|NOT} -in2 subset2
    -out subset
```

To create a subset from a query of the database:

```
$SCHRODINGER/utilities/phasedb_subset -db database {-confs|-sites} {true|false} -out subset
```

To export structures from a database to a file:

```
$SCHRODINGER/utilities/phasedb_export -db database -ofmt basename [-JOB jobname] [-sub subset]
    [-get maxConfs] [-limit maxStruct] [-quota Gbytes] [-gz] [-ext ext] [job-options]
```

To extract properties from a database:

```
$SCHRODINGER/utilities/phasedb_props [job-options] -extract dbName -props propsFile [-csv csvFile]
```

To query properties extracted from a database:

```
$SCHRODINGER/utilities/phasedb_props [job-options] -query string -props propsFile [-sub subsetName]
    [-csv csvFile]
```

To completely remove a database:

```
$SCHRODINGER/utilities/phasedb_manage -delete -db database -all [job-options]
```

To convert a database:

```
$SCHRODINGER/utilities/phasedb_convert -source dbSource -target dbTarget [-new] [-RESTART]
[-fd fdFile] [-records recordFile] [-sites {new|copy|skip}] [-blimit maxMol]
```

To count records in a database or database subset file:

```
$SCHRODINGER/utilities/phasedb_count_records -rec recordsFile [-count countFile]
```

To split a ligand records file for subjob processing:

```
$SCHRODINGER/utilities/phasedb_split_records -rec recordsFile -job jobname -nsub nsub
[-minRec minRec]
```

To check database integrity:

```
$SCHRODINGER/utilities/phasedb_check -db dbName [-blocks_file filename]
```

To back up a database:

```
$SCHRODINGER/utilities/phasedb_recovery -backup -db dbName -db_backup backupName
[-blocks_file fileName] [-add_to_dest]
```

To restore a database from a backup:

```
$SCHRODINGER/utilities/phasedb_recovery -restore -db dbName -db_backup backupName
[-blocks_file fileName]
```

To compact a database:

```
$SCHRODINGER/utilities/phasedb_compact -db dbName [-blocks_file filename]
```

To merge one database into another:

```
$SCHRODINGER/utilities/phasedb_merge -source sourcedbName -dest destinationdbName
```

To add indices for database keys:

```
$SCHRODINGER/utilities/phasedb_index -db dbName
```

To search for matches to 3D keys in a database:

```
$SCHRODINGER/utilities/phasedb_match_keys -db dbName -hypo hypoID [-dtol deltaDist]
[-minSites minSites] [-sub dbSubsetFile] -rec recordsFile
```

To search for matches in a database:

```
$SCHRODINGER/utilities/phasedb_findmatches -setup jobname -db dbName -hypo hypoID -mode runMode
[-sub dbSubset] [-flexSearchMethod {rapid|thorough}] [-flexMaxConfs maxConfs]
[-flexMaxRelEnergy energy] [-flexAmideOption {vary|orig|trans}] [-deltaDist deltaDist]
[-minSites minSites] [-preferBigMatches {true|false}] [-timeLimit timeLimit]
[-useDbKeys {true|false}] [-useExistingSites {true|false}] [-useRefLigand {true|false}]
[-useFeatureRules {true|false}] [-useSiteMask {true|false}] [-useDeltaHypo {true|false}]
[-useFeatureCutoffs {true|false}] [-atomTypeVol {true|false}] [-useExclVol {true|false}]
[-useQSARModel {true|false}] [-alignWeight alignWeight] [-alignCutoff alignCutoff]
[-hardAlignCutoff {true|false}] [-alignPenalty alignPenalty] [-vectorWeight vectorWeight]
[-vectorCutoff vectorCutoff] [-volumeWeight volumeWeight] [-volumeCutoff volumeCutoff]
[-matchFile matchFile] [-writeMatchFile {true|false}] [-maxHits maxHits]
```

```
[ -maxHitsPerMol maxHitsPerMol ]
$SCHRODINGER/phase_dbsearch [job-options] [-BLOCK m] jobname
$SCHRODINGER/utilities/phasedb_findmatches -cleanup jobname
```

To screen a database (or files) by molecular shape:

```
$SCHRODINGER/phase_shape -screen screenSource -shape shapeFile -JOB jobname [job-options]
  {-CHECKPOINT|-RESTART path|-NO_CHECKPOINT} [-title propName] [-filter minSim]
  [-sort [-keep maxKeep]] [-hydrogens] [-atomTypes {mmod|element|pharm}]
  [-flex [-flexSearchMethod {rapid|thorough}] [-flexMaxConfs maxConfs]
  [-flexMaxRelEnergy energy] [-flexAmideOption {vary|orig|trans}]
  [-isub dbSubIn] [-osub dbSubOut] [-HELP]
```

In the commands above, *job-options* represents the standard Job Control options and other job options:

- HOST *host* Run the job on the specified host.
- LOCAL Run the job in the current directory, rather than in a temporary scratch directory.
- TMPDIR *tmpdir* Use *tmpdir* for temporary files.
- WAIT Do not return control to the shell until the job finishes.
- INTERVAL *n* Interval in seconds between output updates.
- NICE Run the job at reduced priority.